

Numerical methods and machine learning algorithms for solution of Inverse problems

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Outline of the course lectures

- **Lecture 1:** Organization of the course. Definitions of well and ill-posed problems. Physical formulations leading to ill- and well-posed problems.
- **Lecture 2:** Compact set and compact operator. Classical and conditional correctness. Concept of Tikhonov and Tikhonov's theorem. Quasi-solution. Examples of ill-posed problems. Model inverse problems: elliptic inverse Cauchy problem.
- **Lecture 3:** Methods for image reconstruction and image deblurring. Solution of a Fredholm integral equation of the first kind as an ill-posed problem. Bayesian approach. Adaptive finite element method in Microwave Imaging for monitoring of hyperthermia.
- **Lecture 4:** Lagrangian approach for solution of time-harmonic CIP. Presentation and discussion of the course project "Solution of time-harmonic acoustic coefficient inverse problem".
- **Lecture 5:** Methods of regularization of inverse problems: Tikhonov's regularization, iterative regularization, Morozov's discrepancy, balancing principle.

- **Lecture 6:** Approximate global convergence and Adaptive finite element method for solution of hyperbolic CIP.
- **Lecture 7:** QR and SVD. Solution of rank-deficient problems. Principal Component Analysis (PCA) for image compression and image recognition. Presentation of the course project "Principal Component Analysis for recognition of handwritten digits".
- **Lecture 8:** Classification algorithms: linear and polynomial classifiers, linear and quadratic perceptron learning algorithm, WINNOW. Neural networks for classification.
- **Lecture 9:** Linear models for regression. Regularized and non-regularized neural networks. Kernel methods. Support Vector Machines. Kernel perceptron for classification. Presentation of the course project "Regularized Least squares and machine learning algorithms for classification problem".
- **Lecture 10:** Lagrangian approach and adaptive FEM for solution of parameter identification problem for system of ODE. Application of adaptive FEM for determination of drug efficacy in the model of HIV infection.

Types of instruction and assessment

- The material of the course includes online lectures in Zoom (slides and video lectures), description of the computer projects and open source software (Matlab codes, C++/PETSC codes).
- All material of the course is available in CANVAS (contact me for registration if you need it):
<https://canvas.gu.se/courses/1223700000000049154>
- Language of instruction is English.
- The grade Pass (G) or Fail (U) is given in this course, and 7.5 Hp.
- The examination consists of the computer project and programs submitted to my mail.

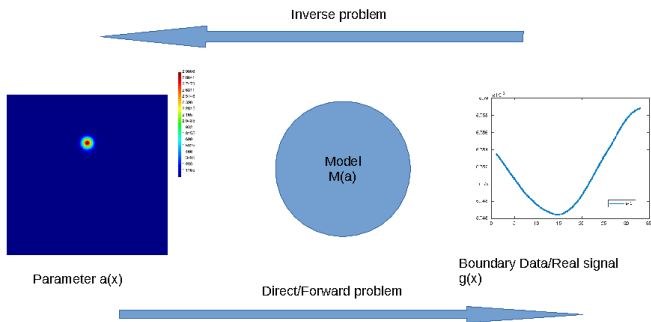
Organization: projects

- To pass this course you should do any computer project described below. The project can be done in groups by 2-4 persons, or you can do it without group as well.
- Sent final report for computer project with description of your work together with Matlab or C++/PETSc programs. For students registered at Chalmers/GU: download projects in CANVAS, for all others: sent project to my e-mail larisa@chalmers.se
- Report should be organized as scientific paper and have description of used techniques, tables and figures confirming your investigations. Analysis of obtained results is necessary to present in section “Numerical examples” and summarize results in the section “Conclusion”.

List of the course projects

- 1. Project "*Regularized least squares and machine learning algorithms for classification*". Matlab program with an example of classification of Iris dataset see in CANVAS in "Computer Projects".
- 2. Project "*Principal component analysis for image recognition*". Matlab program with an example of using PCA see in CANVAS in "Computer Projects".
- 3. Project "*Solution of time-harmonic acoustic coefficient inverse problem*". Matlab code with an example of solution of Poisson's equation in 2D see in CANVAS in "Computer Projects". C++/PETSc code is in waves24.com/download
- 4. Project "*Regularized algorithms for detection of tumours in microwave medical imaging*". Matlab code (data and programs, zip file) with an example see in CANVAS in "Computer Projects".
- 5* **Alternative project with extended deadline: "SVM and Kernel methods for classification"** (similar to the first project, but SVM and Kernel methods should be applied). There is no example in Matlab, but perhaps, you can modify the example with Iris dataset for classification from the above project.

Introduction: Inverse and ill-posed problems

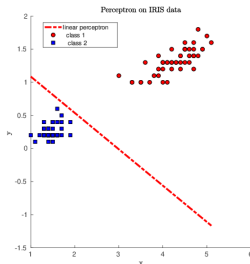
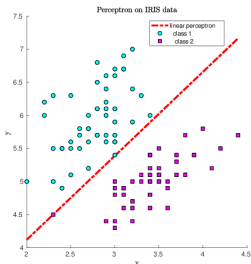


Example: Scheme for solution of CIP for $\Delta u(x) - s^2 a(x)u(x) = -f(x), \partial_n u = 0$.

- Inverse and ill-posed problems include solution of CIPs for PDE, solution of parameter identification problems governed by system of ODE, inverse source problems, inverse spectral problems, solution of Fredholm integral equations of the first kind (ill-posed problems).

Classification problems

Classification problems can be considered as the type of inverse problem since the goal of classification is to find optimal vector of weights $\omega = [\omega_1, \dots, \omega_n]$ to separate given data x by the decision line $\omega^T x$.



Example of classification: determine the decision line for points presented in the Figure. Two classes are separated by the linear equation with three weights $\omega_i, i = 1, 2, 3$, given by

$$\omega_1 + \omega_2 x + \omega_3 y = 0. \quad (1)$$

Decision lines on the figure computed by the perceptron learning algorithm for separation of two classes using Iris dataset.

Test Matlab program to generate this figures on the course page in CANVAS.



Classical Correctness and Conditional Correctness

The notion of the classical correctness is called sometimes *Correctness by Hadamard*.

Definition. Let B_1 and B_2 be two Banach spaces. Let $G \subseteq B_1$ be an open set and $F : G \rightarrow B_2$ be an operator. Consider the equation

$$F(x) = y, \quad x \in G. \quad (2)$$

The problem of solution of equation (2) is called *well-posed by Hadamard*, or simply *well-posed*, or *classically well-posed* if the following three conditions are satisfied:

1. For any $y \in B_2$ there exists a solution $x = x(y)$ of equation (2) (existence theorem).
2. This solution is unique (uniqueness theorem).
3. The solution $x(y)$ depends continuously on y . In other words, the operator $F^{-1} : B_2 \rightarrow B_1$ is continuous.

If equation (2) does not satisfy to at least one these three conditions, then the problem (2) is called *ill-posed*.

Introduction: Inverse and ill-posed problems

- The theory of Ill-Posed Problems addresses the following fundamental question: *How to obtain a good approximation for the solution of an ill-posed problem in a stable way?*
- A numerical method, which provides a stable and accurate solution of an ill-posed problem, is called the *regularization* method for this problem.
- Foundations of the theory of Ill-Posed Problems were established by A. N. Tikhonov [T1,TA,T], M.M. Lavrent'ev [L] and V. K. Ivanov [I] in 1960-ies. The first foundational work was published by Tikhonov in 1943 [T].

[T1] A. N. Tikhonov, On the stability of inverse problems, *Doklady of the USSR Academy of Science*, 39, 195-198, 1943

[TA] A. N. Tikhonov and V. Y. Arsenin. *Solutions of Ill-Posed Problems*, Winston and Sons, Washington, DC, 1977.

[T] A.N. Tikhonov, A.V. Goncharsky, V.V. Stepanov and A.G. Yagola, *Numerical Methods for the Solution of Ill-Posed Problems*, London: Kluwer, London, 1995.

[L] M.M. Lavrentiev, *Some Improperly Posed Problems of Mathematical Physics*, Springer, New York, 1967.

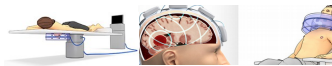
[I] V. K. Ivanov, On ill-posed problems, *Mat. USSR Sb.*, 61, 211–223, 1963.

Introduction: Inverse and ill-posed problems

- Theory of inverse and ill-posed problems is developed further and a lot of new works on this subject are available, some of them are:
 - S. Arridge, Optical tomography in medical imaging, *Inverse Problems*, 15, 841–893, 1999.
 - A.B. Bakushinsky and M.Yu. Kokurin, *Iterative Methods for Approximate Solution of Inverse Problems*, Springer, New York, 2004.
 - F. Cakoni and D. Colton, *Qualitative Methods in Inverse Scattering Theory*, Springer, New York, 2006.
 - K. Chadan and P. Sabatier, *Inverse Problems in Quantum Scattering Theory*, Springer, New York, 1989.
 - G. Chavent, *Nonlinear Least Squares for Inverse Problems: Theoretical Foundations and Step-by-Step Guide for Applications (Scientific Computation)*, Springer, New York, 2009.
 - V. Isakov, *Inverse Problems for Partial Differential Equations*, Springer, New York, 2005.
 - B. Kaltenbacher, A. Neubauer and O. Scherzer, *Iterative Regularization Methods for Nonlinear Ill-Posed Problems*, de Gruyter, New York, 2008.
 - A. Kirsch, *An Introduction To the Mathematical Theory of Inverse Problems*, Springer, New York, 2011.
 - K. Ito, B. Jin, *Inverse Problems: Tikhonov theory and algorithms*, Series on Applied Mathematics, V.22, World Scientific, 2015.
 - Tikhonov, A.N., Goncharsky, A., Stepanov, V.V., Yagola, A.G., *Numerical Methods for the Solution of Ill-Posed Problems*, ISBN 978-94-015-8480-7, 1995.

Applications leading to inverse and ill-posed problems

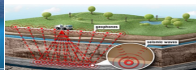
Microwave medical imaging



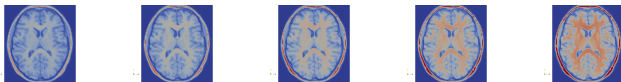
Acoustic imaging



Elastic imaging



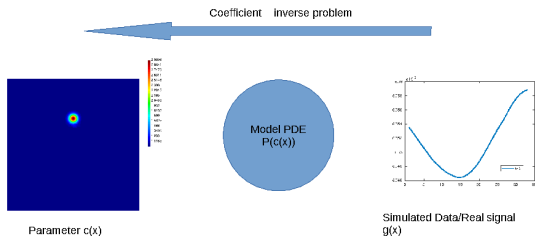
Examples of CIPs. Biomedical Imaging at the Department of Electrical Engineering at CTH, Chalmers. Left: breast cancer detection, setup of Stroke Finder; microwave hyperthermia in cancer treatment; Middle: acoustic imaging; right: subsurface imaging.



Example of ill-posed problem: restoration of MRI images for the parietal lobe <http://brain-development.org/>

- Inverse and ill-posed problems arise in many real-world applications including medical microwave, optical and ultrasound imaging, MRT, MRI, oil prospecting and shape reconstruction, nondestructive testing of materials and detection of explosives, seeing through the walls and constructing of new materials.
- Physical applications are modelled by acoustic, elastic or electromagnetic wave eq. which include different physical parameters s , t , wave speed c - acoustic equation; elasticity parameters λ and μ - elastic equations; dielectric permittivity ϵ , magnetic permeability μ , conductivity σ - Maxwell's eq.
- A **coefficient inverse problem** for a given model PDE aims at estimating a spatially distributed coefficient of the model PDE using measurements taken on the boundary of the domain of interest.

Introduction: Inverse and ill-posed problems

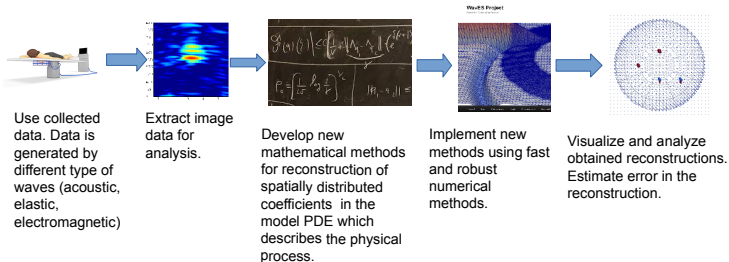


- These applications are modeled by acoustic, elastic or electromagnetic wave eq. which include different physical parameters (wave speed c - acoustic equation, elasticity parameters λ and μ - elastic equations, dielectric permittivity ε , magnetic permeability μ , conductivity σ - Maxwell's eq.).
- A **coefficient inverse problem** for a given PDE aims at estimating a spatially distributed coefficient of the model PDE using measurements taken on the boundary of the domain of interest.

Coefficient Inverse Problems: main steps in solution

Coefficient Inverse Problems for PDE

A coefficient inverse problem for a given partial differential equation (PDE) aims at estimating a spatially distributed coefficient of the model PDE using measurements taken on the boundary of the domain of interest.



- **Acoustic CIPs** for acoustic wave equation

$$\frac{1}{c^2(x)} u_{tt} = \Delta u \text{ in } \mathbb{R}^3 \times (0, \infty), \quad (3)$$

$$u(x, 0) = 0, u_t(x, 0) = \delta(x - x_0). \quad (4)$$

- Let now introduce the convex bounded domain $\Omega \subset \mathbb{R}^3$ with the boundary $\partial\Omega \in C^3$ and specify time variable $t \in [0, T]$. Next, we supply the Cauchy problem by the appropriate b.c.
- We assume that the coefficient $c(x)$ belongs to the set of admissible parameters M which should be specified for the concrete problem.
- $u(x, t)$ acoustic pressure - we measure it on the boundary $\partial\Omega$.
- $c(x)$ speed of sound – want to determine by measured $u(x, t)$ on the boundary $\partial\Omega$
- Applications: medical imaging, electromagnetic, acoustics, geological profiling, construction of new materials

Acoustic CIP: example

We model the process of electric wave field propagation in non-conductive and nonmagnetic media with $\nabla \cdot (\varepsilon E) = 0$ via a single hyperbolic PDE, which is the same as an acoustic wave equation (3)-(4). The forward problem is the following Cauchy problem

$$\varepsilon_r(x)u_{tt} = \Delta u, \text{ in } \mathbb{R}^3 \times (0, \infty), \quad (5)$$

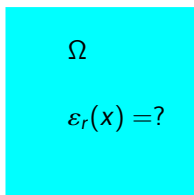
$$u(x, 0) = 0, \quad u_t(x, 0) = \delta(x - x_0). \quad (6)$$

Here, $\varepsilon_r(x)$ is the spatially distributed dielectric constant (relative dielectric permittivity),

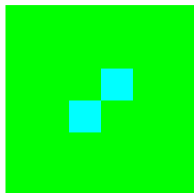
$$\varepsilon_r(x) = \frac{\varepsilon(x)}{\varepsilon_0}, \quad \sqrt{\varepsilon_r(x)} = n(x) = \frac{c_0}{c(x)} \geq 1, \quad (7)$$

where ε_0 is the dielectric permittivity of the vacuum (which we assume to be the same as the one in the air), $\varepsilon(x)$ is the dielectric permittivity of the medium of interest, $n(x)$ is the refractive index of the medium of interest, $c(x)$ is the speed of the propagation of the EM field in this medium, and c_0 is the speed of light in the vacuum, which we assume to be the same as one in the air.

Acoustic CIP: example



$$u(x, t) = g(x, t) \text{ on } \partial\Omega$$

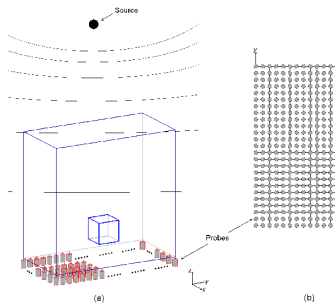


$$\text{exact } \varepsilon_r(x)$$

Coefficient Inverse Problem Assume that the function $\varepsilon_r(x)$ is unknown in the domain Ω . Determine the function $\varepsilon_r(x)$ for $x \in \Omega$, assuming that the following function $g(x, t)$ is known for a source $x_0 \notin \bar{\Omega}$

$$u(x, t) = g(x, t), \forall (x, t) \in \partial\Omega \times (0, T].$$

Reconstruction of dielectrics from experimental data



a) The rectangular prism depicts our computational domain Ω . Only a single source location outside of this prism was used. Tomographic measurements of the scattered time resolved EM wave were conducted on the bottom side of this prism. The signal was measured with the time interval 20 picoseconds with total time 12.3 nanoseconds. b) Schematic diagram of locations of detectors on the bottom side of the prism Ω . The distance between neighboring detectors was 10 mm.

L.Beilina, M.V.Klibanov, Reconstruction of dielectrics from experimental data via a hybrid globally convergent/adaptive inverse algorithm, *Inverse Problems*, 26, 125009, 2010.

The two-stage numerical procedure for solution of CIP

Stage 1. Approximately globally convergent numerical method provides a good approximation for the exact solution ε_{glob} .

Stage 2. Adaptive Finite Element Method refines it via minimization of the corresponding Tikhonov functional with $\varepsilon_0 = \varepsilon_{glob}$:

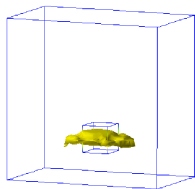
$$J(u, \varepsilon) = \frac{1}{2} \int_{\Gamma} \int_0^T (u - \tilde{u})^2 z_{\delta}(t) ds dt + \frac{1}{2} \gamma \int_{\Omega} (\varepsilon - \varepsilon_0)^2 dx. \quad (8)$$

where \tilde{u} is the observed wave field in the model PDE (for example, acoustic wave equation), u satisfies this model PDE and thus depends on ε .

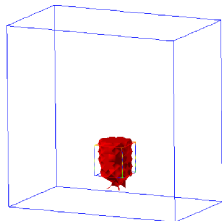
The two-stage numerical procedure

Stage 1. Approximately globally convergent numerical method provides a good approximation for the exact solution.

Stage 2. Adaptive Finite Element Method refines it.



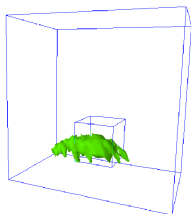
$$\text{a) } \varepsilon_r^{(5,2)} = 3.9, n^{(5,2)} = 1.97$$



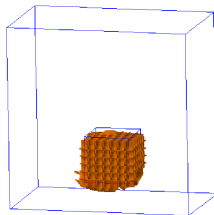
$$\text{b) } \varepsilon_{r,h} \approx 4.2, n_{glob} = \sqrt{\varepsilon_{r,h}} \approx 2.05$$

a) A sample of the reconstruction result of the dielectric cube No. 1 (4 cm side) via the first stage. b) Result after applying the adaptive stage (2-nd stage). The side of the cube is 4 cm=1.33 wavelength.

Results of the two-stage procedure, cube nr.2 (big)



a) $\varepsilon_r(5,5) = 3.19, n^{(5,5)} = 1.79$



b) $\varepsilon_{r,h} \approx 3.0, n_{glob} = \sqrt{\varepsilon_{r,h}} \approx 1.73$

a) Reconstruction of the dielectric cube No. 2 (6 cm side) via the first stage. b) The final reconstruction result after applying the adaptive stage (2-nd stage). The side 6 cm=2 wavelength.

L.Beilina, M.V.Klibanov, Reconstruction of dielectrics from experimental data via a hybrid globally convergent/adaptive inverse algorithm, *Inverse Problems*, 26, 125009, 2010.

Let $v(x, t) = (v_1, v_2, v_3)(x, t)$ be vector of displacement. We consider the Cauchy problem for the elastodynamics equations in the isotropic case in the entire space \mathbb{R}^3 ,

$$\begin{aligned}\rho(x) \frac{\partial^2 v}{\partial t^2} - \nabla \cdot \tau &= \delta(x_3 - z_0) f(t), \\ \tau &= C \epsilon,\end{aligned}\tag{9}$$

$$v(x, 0) = 0, v_t(x, 0) = 0, \quad x \in \mathbb{R}^3, t \in (0, T),$$

where $v(x, t)$ is the total displacement generated by the incident plane wave $f(t)$ propagating along the x_3 -axis which is incident at the plane $x_3 = z_0$, $\rho(x)$ is the density of the material, τ is the stress tensor, C is a cyclic symmetric tensor and ϵ is the strain tensor which have components

$$\epsilon_{ij} = \frac{1}{2} \left(\frac{\partial v_i}{\partial x_j} + \frac{\partial v_j}{\partial x_i} \right), \quad i, j = 1, 2, 3.$$

The strain tensor ϵ is coupled with the stress tensor τ by the Hooke's law

$$\tau_{i,j} = \sum_{k=1}^3 \sum_{l=1}^3 C_{ijkl} \epsilon_{kl}\tag{10}$$

C is a cyclic symmetric tensor

$$C_{ijkl} = C_{klij} = C_{jkli}.$$

When C_{ijkl} does not depend on \mathbf{x} then material of the domain which we consider is said to be **homogeneous**. If the tensor C_{ijkl} does not depend on the choice of the coordinate system, then the material of the domain under interest is said to be **isotropic**. Otherwise, the material is **anisotropic**.

In the **isotropic** case the cyclic symmetric tensor C can be written as

$$C_{ijkl} = \lambda \delta_{ij} \delta_{kl} + \mu (\delta_{ij} \delta_{kl} + \delta_{il} \delta_{jk}),$$

where δ_{ij} is the Kronecker delta, in which case the equation (10) takes the form

$$\tau_{i,j} = \lambda \delta_{ij} \sum_{k=1}^3 \epsilon_{kk} + 2\mu \epsilon_{ij}, \quad (11)$$

where λ and μ are **Lame coefficients**.

Lame coefficients λ and μ are given by

$$\begin{aligned}\mu &= \frac{E}{2(1 + \nu)}, \\ \lambda &= \frac{E\nu}{(1 + \nu)(1 - 2\nu)}.\end{aligned}\tag{12}$$

Here, E is the **modulus of elasticity**, or **Young modulus**, and ν is the **Poisson's ratio** of the elastic material. Following relations should be satisfied

$$\lambda > 0, \mu > 0 \iff E > 0, 0 < \nu < 1/2.\tag{13}$$

To write the equation (9) only in terms of v we eliminate the strain tensor ϵ from (9) using (10). Then in the isotropic case the equation in (9) writes

$$\begin{aligned}
 \rho(x) \frac{\partial^2 v_1}{\partial t^2} - \frac{\partial}{\partial x_1} \left((\lambda + 2\mu) \frac{\partial v_1}{\partial x_1} + \lambda \frac{\partial v_2}{\partial x_2} + \lambda \frac{\partial v_3}{\partial x_3} \right) \\
 - \frac{\partial}{\partial x_2} \left(\mu \left(\frac{\partial v_1}{\partial x_2} + \frac{\partial v_2}{\partial x_1} \right) \right) - \frac{\partial}{\partial x_3} \left(\mu \left(\frac{\partial v_1}{\partial x_3} + \frac{\partial v_3}{\partial x_1} \right) \right) &= 0, \\
 \rho(x) \frac{\partial^2 v_2}{\partial t^2} - \frac{\partial}{\partial x_2} \left((\lambda + 2\mu) \frac{\partial v_2}{\partial x_2} + \lambda \frac{\partial v_1}{\partial x_1} + \lambda \frac{\partial v_3}{\partial x_3} \right) \\
 - \frac{\partial}{\partial x_1} \left(\mu \left(\frac{\partial v_1}{\partial x_2} + \frac{\partial v_2}{\partial x_1} \right) \right) - \frac{\partial}{\partial x_3} \left(\mu \left(\frac{\partial v_2}{\partial x_3} + \frac{\partial v_3}{\partial x_2} \right) \right) &= 0, \\
 \rho(x) \frac{\partial^2 v_3}{\partial t^2} - \frac{\partial}{\partial x_3} \left((\lambda + 2\mu) \frac{\partial v_3}{\partial x_3} + \lambda \frac{\partial v_2}{\partial x_2} + \lambda \frac{\partial v_1}{\partial x_1} \right) \\
 - \frac{\partial}{\partial x_2} \left(\mu \left(\frac{\partial v_3}{\partial x_2} + \frac{\partial v_2}{\partial x_3} \right) \right) - \frac{\partial}{\partial x_1} \left(\mu \left(\frac{\partial v_1}{\partial x_3} + \frac{\partial v_3}{\partial x_1} \right) \right) &= \delta(x_3 - z_0) f(t),
 \end{aligned} \tag{14}$$

The system above for $\lambda = \text{const.} > 0, \mu = \text{const.} > 0$ can be written in a more compact form as

$$\rho \frac{\partial^2 \mathbf{v}}{\partial t^2} - \mu \nabla \cdot (\nabla \mathbf{v}) - (\lambda + \mu) \nabla (\nabla \cdot \mathbf{v}) = \delta(x_3 - z_0) f(t),$$
$$\mathbf{v}(x, 0) = 0, v_i(x, 0) = 0, \quad x \in \mathbb{R}^3, t \in (0, T).$$
(15)

Inserting Helmholtz decomposition

$$\mathbf{v} = \nabla \varphi + \nabla \times \psi$$
(16)

with a scalar potential φ and a vector potential ψ into (15) we get

$$\rho \frac{\partial^2 (\nabla \varphi + \nabla \times \psi)}{\partial t^2} - \mu \nabla \cdot (\nabla (\nabla \varphi + \nabla \times \psi)) - (\lambda + \mu) \nabla (\nabla \cdot (\nabla \varphi + \nabla \times \psi))$$
$$= \delta(x_3 - z_0) f(t)$$
(17)

Using

$$\begin{aligned}\nabla \cdot (\nabla \varphi) &= \Delta \varphi, \\ \nabla \cdot (\nabla \times \psi) &= 0,\end{aligned}$$

we finally get with $f(t) = 0$

$$\nabla \left(\rho \frac{\partial^2 \varphi}{\partial t^2} - (\lambda + 2\mu) \Delta \varphi \right) + \nabla \times \left(\rho \frac{\partial^2 \psi}{\partial t^2} - \mu \Delta \psi \right) = 0 \quad (18)$$

We conclude that

$$\begin{aligned}\rho \frac{\partial^2 \varphi}{\partial t^2} - (\lambda + 2\mu) \Delta \varphi &= 0, \\ \rho \frac{\partial^2 \psi}{\partial t^2} - \mu \Delta \psi &= 0.\end{aligned} \quad (19)$$

Here, $v = \nabla \varphi$ is the pressure wave with the speed $V_p = \left(\frac{\lambda + 2\mu}{\rho} \right)^{1/2}$,
 $v = \nabla \times \psi$ is the shear wave with the speed $V_s = \left(\frac{\mu}{\rho} \right)^{1/2}$

Ω

$$\rho(x) = ?$$

$$\lambda(x), \mu(x) \in \Omega$$

$$u(x, t) = g(x, t) \text{ on } \partial\Omega$$

 Ω

$$\left. \begin{aligned} \rho(x) &= ? \\ \lambda(x) &= ? \end{aligned} \right\}$$

$$\mu(x) = ?$$

$$v(x, t) = g(x, t) \text{ on } \partial\Omega$$

Inverse Problem (IP1) Determine the density function $\rho(x)$ in Ω for $x \in \Omega$ assuming that the Lamé parameters $\lambda(x), \mu(x)$ and $g(x, t)$ s.t.

$$v(x, t) = g(x, t), \forall (x, t) \in \partial\Omega \times (0, T].$$

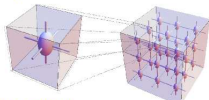
are known in Ω .

Inverse Problem (IP2) Determine the functions $\rho(x), \lambda(x), \mu(x)$ in Ω for $x \in \Omega$ assuming that $g(x, t)$ is known in Ω .

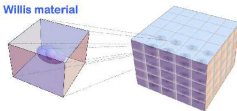
Applications of elastic CIP: design of new materials

There is a class of materials for which the macroscale properties can be obtained more from such called mechanical *microstructural* design, see Figure for examples of such materials.

Micropolar material



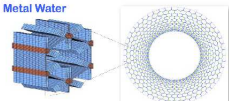
Willis material



Auxetic material



Metal Water



- Practical applications: mechanical cloaking, control and manipulation of waves in fluids and solids, etc.
- Examples of such materials include nanomaterials such as graphene or carbon nanotubes with extraordinary strength properties.
- Design of new mechanical metamaterials using computational modeling is one of the applications of elastic CIPs.

CIP for electromagnetic problems. Maxwell's equations

Consider a region of space that has no electric or magnetic current sources, but may have materials that absorb electric or magnetic field energy. Then, using MKS units, the time-dependent Maxwell's equations are given in **differential** and **integral** form by *Faraday's law* :

$$\frac{\partial \mathbf{B}}{\partial t} = -\nabla \times \mathbf{E} - \mathbf{M} \quad (20a)$$

$$\frac{\partial}{\partial t} \iint_A \mathbf{B} \cdot d\mathbf{A} = - \oint_L \mathbf{E} \cdot d\mathbf{L} - \iint_A \mathbf{M} \cdot d\mathbf{A} \quad (20b)$$

The MKS system of units is a physical system of units that expresses any given measurement using fundamental units of the metre, kilogram, and/or second (MKS))

Maxwell's equations

Ampere's law :

$$\frac{\partial \mathbf{D}}{\partial t} = \nabla \times \mathbf{H} - \mathbf{J} \quad (21a)$$

$$\frac{\partial}{\partial t} \iint_A \mathbf{D} \cdot d\mathbf{A} = \oint_L \mathbf{H} \cdot d\mathbf{L} - \iint_A \mathbf{J} \cdot d\mathbf{A} \quad (21b)$$

Gauss' law for the electric field :

$$\nabla \cdot \mathbf{D} = 0 \quad (22a)$$

$$\oiint_A \mathbf{D} \cdot d\mathbf{A} = 0 \quad (22b)$$

Gauss' law for the magnetic field :

$$\nabla \cdot \mathbf{B} = 0 \quad (23a)$$

$$\oiint_A \mathbf{B} \cdot d\mathbf{A} = 0 \quad (23b)$$

Maxwell's equations

In (20) to (23), the following symbols (and their MKS units) are defined:

- E** : electric field (volts/meter)
- D** : electric flux density (coulombs/meter²)
- H** : magnetic field (amperes/meter)
- B** : magnetic flux density (webers/meter²)
- A** : arbitrary three-dimensional surface
- dA** : differential normal vector that characterizes surface *A* (meter²)
- L** : closed contour that bounds surface *A* (volts/meter)
- dL** : differential length vector that characterizes contour *L* (meters)
- J** : electric current density (amperes/meter²)
- M** : equivalent magnetic current density (volts/meter²)

Maxwell's equations

In linear, isotropic, nondispersive materials (i.e. materials having field-independent, direction-independent, and frequency-independent electric and magnetic properties), we can relate \mathbf{D} to \mathbf{E} and \mathbf{B} to \mathbf{H} using simple proportions:

$$\mathbf{D} = \varepsilon \mathbf{E} = \varepsilon_r \varepsilon_0 \mathbf{E}; \quad \mathbf{B} = \mu \mathbf{H} = \mu_r \mu_0 \mathbf{H} \quad (24)$$

where

- ε : electrical permittivity (farads/meter)
- ε_r : relative permittivity (dimensionless scalar)
- ε_0 : free-space permittivity (8.854×10^{-12} farads/meter)
- μ : magnetic permeability (henrys/meter)
- μ_r : relative permeability (dimensionless scalar)
- μ_0 : free-space permeability ($4\pi \times 10^{-7}$ henrys/meter)

Note that \mathbf{J} and \mathbf{M} can act as *independent sources* of E- and H-field energy, \mathbf{J}_{source} and \mathbf{M}_{source} .

Maxwell's equations

We also allow for materials with isotropic, nondispersive electric and magnetic losses that attenuate E- and H-fields via conversion to heat energy. This yields

$$\mathbf{J} = \mathbf{J}_{source} + \sigma \mathbf{E}; \quad \mathbf{M} = \mathbf{M}_{source} + \sigma^* \mathbf{H} \quad (25)$$

where σ : electric conductivity (siemens/meter)
 σ^* : equivalent magnetic loss (ohms/meter)

Finally, we substitute (24) and (25) into (20a) and (21a). This yields Maxwell's curl equations in linear, isotropic, nondispersive, lossy materials:

$$\frac{\partial \mathbf{H}}{\partial t} = -\frac{1}{\mu} \nabla \times \mathbf{E} - \frac{1}{\mu} (\mathbf{M}_{source} + \sigma^* \mathbf{H}) \quad (26)$$

$$\frac{\partial \mathbf{E}}{\partial t} = \frac{1}{\varepsilon} \nabla \times \mathbf{H} - \frac{1}{\varepsilon} (\mathbf{J}_{source} + \sigma \mathbf{E}) \quad (27)$$

Maxwell's equations

We now write out the vector components of the curl operators of (26) and (27) in Cartesian coordinates. This yields the following system of six coupled scalar equations:

$$\frac{\partial H_x}{\partial t} = \frac{1}{\mu} \left[\frac{\partial E_y}{\partial z} - \frac{\partial E_z}{\partial y} - (M_{source_x} + \sigma^* H_x) \right] \quad (28a)$$

$$\frac{\partial H_y}{\partial t} = \frac{1}{\mu} \left[\frac{\partial E_z}{\partial x} - \frac{\partial E_x}{\partial z} - (M_{source_y} + \sigma^* H_y) \right] \quad (28b)$$

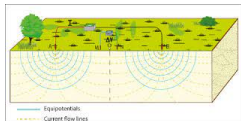
$$\frac{\partial H_z}{\partial t} = \frac{1}{\mu} \left[\frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} - (M_{source_z} + \sigma^* H_z) \right] \quad (28c)$$

$$\frac{\partial E_x}{\partial t} = \frac{1}{\varepsilon} \left[\frac{\partial H_z}{\partial y} - \frac{\partial H_y}{\partial z} - (J_{source_x} + \sigma E_x) \right] \quad (29a)$$

$$\frac{\partial E_y}{\partial t} = \frac{1}{\varepsilon} \left[\frac{\partial H_x}{\partial z} - \frac{\partial H_z}{\partial x} - (J_{source_y} + \sigma E_y) \right] \quad (29b)$$

$$\frac{\partial E_z}{\partial t} = \frac{1}{\varepsilon} \left[\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} - (J_{source_z} + \sigma E_z) \right] \quad (29c)$$

Maxwell's equations in electrical prospecting



- CIPs of electrical prospecting appears in subsurface imaging. The CIP is as follows: the electromagnetic field is measured on the surface of the ground. The problem is to find the electric conductivity σ and magnetic permeability μ of the geological medium.
- To formulate the forward problem in frequency domain we will apply the Fourier transform in time to the full system of Maxwell's equations such that the time-harmonic fields $\mathbf{A}(x, \omega)$ are initialized in the form

$$\mathbf{A}(x, \omega) = \int_0^{\infty} \mathbf{A}(x, t) e^{-i\omega t} dt. \quad (30)$$

Maxwell's equations in electrical prospecting

We will use Sommerfeld radiation condition at infinity for $A(x, \omega)$:

$$\lim_{|x| \rightarrow \infty} |x|^{\frac{n-1}{2}} \left(\frac{\partial}{\partial |x|} + ik \right) A = 0, \quad n = 2, 3. \quad (31)$$

where k is the wave number,

Maxwell's equations in electrical prospecting

Now, we apply (30) to the system (26)-(27). We multiply system (26)-(27) with $\exp^{-i\omega t}$ and integrate it in time to get

$$\begin{aligned}\int_0^{+\infty} \frac{\partial \mathbf{H}}{\partial t} \exp^{-i\omega t} dt &= -\frac{1}{\mu} \int_0^{+\infty} \nabla \times \mathbf{E} \exp^{-i\omega t} dt \\ &\quad - \frac{1}{\mu} \left(\int_0^{+\infty} \mathbf{M}_{source} \exp^{-i\omega t} dt + \sigma^* \int_0^{+\infty} \mathbf{H} \exp^{-i\omega t} dt \right) \\ \int_0^{+\infty} \frac{\partial \mathbf{E}}{\partial t} \exp^{-i\omega t} dt &= \frac{1}{\varepsilon} \int_0^{+\infty} \nabla \times \mathbf{H} \exp^{-i\omega t} dt \\ &\quad - \frac{1}{\varepsilon} \left(\int_0^{+\infty} \mathbf{J}_{source} \exp^{-i\omega t} dt + \sigma \int_0^{+\infty} \mathbf{E} \exp^{-i\omega t} dt \right)\end{aligned}\tag{32}$$

In this system we consider $\mathbf{M}_{source} = 0$, $\sigma^* = 0$, $\mathbf{J}_{source} = 0$ in accordance with applications in electrical prospecting.

Maxwell's equations in electrical prospecting

In this (32) we consider $\mathbf{M}_{source} = 0, \sigma^* = 0, \mathbf{J}_{source} = 0$ in accordance with applications in electrical prospecting such that the above system is reduced to the system

$$\begin{aligned}\int_0^{+\infty} \frac{\partial \mathbf{H}}{\partial t} \exp^{-i\omega t} dt &= -\frac{1}{\mu} \int_0^{+\infty} \nabla \times \mathbf{E} \exp^{-i\omega t} dt \\ \int_0^{+\infty} \frac{\partial \mathbf{E}}{\partial t} \exp^{-i\omega t} dt &= \frac{1}{\varepsilon} \int_0^{+\infty} \nabla \times \mathbf{H} \exp^{-i\omega t} dt - \frac{1}{\varepsilon} \sigma \int_0^{+\infty} \mathbf{E} \exp^{-i\omega t} dt\end{aligned}\tag{33}$$

Maxwell's equations in electrical prospecting

Next, we integrate by parts in time integrals $\int_0^{+\infty} \frac{\partial \mathbf{H}}{\partial t} \exp^{-i\omega t} dt$ and $\int_0^{+\infty} \frac{\partial \mathbf{E}}{\partial t} \exp^{-i\omega t} dt$ to obtain

$$\begin{aligned} \int_0^{+\infty} \frac{\partial \mathbf{H}}{\partial t} \exp^{-i\omega t} dt &= \exp^{-i\omega t} \mathbf{H} \Big|_0^{+\infty} \\ &\quad + i\omega \int_0^{+\infty} \mathbf{H} \exp^{-i\omega t} dt = i\omega \mathbf{H}(x, \omega) \\ \int_0^{+\infty} \frac{\partial \mathbf{E}}{\partial t} \exp^{-i\omega t} dt &= \exp^{-i\omega t} \mathbf{E} \Big|_0^{+\infty} \\ &\quad + i\omega \int_0^{+\infty} \mathbf{E} \exp^{-i\omega t} dt = i\omega \mathbf{E}(x, \omega) \end{aligned} \tag{34}$$

and substitute them into (33) to obtain

$$\begin{aligned}i\omega\mu \mathbf{H}(x, \omega) &= -\nabla \times \mathbf{E}(x, \omega) \\i\omega\varepsilon \mathbf{E}(x, \omega) &= \nabla \times \mathbf{H}(x, \omega) - \sigma\mathbf{E}(x, \omega)\end{aligned}\tag{35}$$

The above system can be rewritten as

$$\begin{aligned}\nabla \times \mathbf{E}(x, \omega) &= -i\omega\mu \mathbf{H}(x, \omega) \\ \nabla \times \mathbf{H}(x, \omega) &= (i\omega\varepsilon + \sigma)\mathbf{E}(x, \omega)\end{aligned}\tag{36}$$

According to our applications we assume that $\mu = \text{const.}$,
 $\varepsilon = \text{const.} > 0$. We introduce new variable $\sigma_\omega := i\omega\varepsilon + \sigma$ to obtain

$$\begin{aligned}\nabla \times \mathbf{E}(x, \omega) &= -i\omega\mu \mathbf{H}(x, \omega) \\ \nabla \times \mathbf{H}(x, \omega) &= \sigma_\omega \mathbf{E}(x, \omega)\end{aligned}\tag{37}$$

Taking operator of $\nabla \times$ from the first equation in system (37) we have

$$\nabla \times \nabla \times \mathbf{E}(x, \omega) = -i\omega\mu \nabla \times \mathbf{H}(x, \omega) \quad (38)$$

Substituting the second equation of the system (37) in the right hand side of (38) we obtain

$$\nabla \times \nabla \times \mathbf{E}(x, \omega) = -i\omega\mu \sigma_\omega \mathbf{E}(x, \omega) \quad (39)$$

Coefficient Inverse Problem

Let the function $\sigma_\omega(x) \in C^1(\mathbf{R}^3)$, $x \in \mathbf{R}^3$. Let $\Omega \subset \mathbf{R}^3$ be a convex bounded domain with the boundary $\partial\Omega \in C^3$. Determine the coefficient $\sigma_\omega(x) \in \Omega$ assuming that the following function $g(x, \omega)$ is known

$$\mathbf{E}(x, \omega)|_{\partial\Omega} = g(x, \omega) \quad \forall(x, \omega) \in \partial\Omega \times (0, +\infty) \quad (40)$$

CIPs for electric wave propagation

Recall Maxwell's curl equations in linear, isotropic, nondispersive, lossy materials with $\sigma^* = 0$, $\mathbf{M}_{source} = 0$:

$$\frac{\partial \mathbf{H}}{\partial t} = -\frac{1}{\mu} \nabla \times \mathbf{E} \quad (41)$$

$$\frac{\partial \mathbf{E}}{\partial t} = \frac{1}{\varepsilon} \nabla \times \mathbf{H} - \frac{1}{\varepsilon} \sigma \mathbf{E} - \frac{1}{\varepsilon} \mathbf{J}_{source} \quad (42)$$

Take now $\frac{\partial}{\partial t}$ from (42) and $\nabla \times$ from (41) to get:

$$\nabla \times \frac{\partial \mathbf{H}}{\partial t} = -\nabla \times \frac{1}{\mu} \nabla \times \mathbf{E} \quad (43)$$

$$\varepsilon \frac{\partial^2 \mathbf{E}}{\partial t^2} = \frac{\partial}{\partial t} \nabla \times \mathbf{H} - \sigma \frac{\partial \mathbf{E}}{\partial t} - \frac{\partial \mathbf{J}_{source}}{\partial t} \quad (44)$$

CIPs for electric wave propagation

Substitute the right hand side of (43) into (44) instead of $\frac{\partial}{\partial t} \nabla \times \mathbf{H}$ to obtain Maxwell's equations for electric field $\mathbf{E} = (E_1, E_2, E_3)$. Let us consider now Cauchy problem for the Maxwell's equations for electric field \mathbf{E} in the domain $\Omega_T = \Omega \times [0, T]$:

$$\begin{aligned} \varepsilon \frac{\partial^2 \mathbf{E}}{\partial t^2} + \nabla \times \frac{1}{\mu} \nabla \times \mathbf{E} &= -\sigma \frac{\partial \mathbf{E}}{\partial t} - \frac{\partial}{\partial t} \mathbf{J}_{source} \text{ in } \Omega_T, \\ \nabla \cdot (\varepsilon \mathbf{E}) &= 0, \end{aligned} \tag{45}$$

$$\mathbf{E}(\mathbf{x}, \mathbf{0}) = f_0(x), \quad \mathbf{E}_t(\mathbf{x}, \mathbf{0}) = f_1(x) \text{ in } \Omega,$$

- Let $\Omega \subset \mathbb{R}^3$ be a convex bounded domain with the boundary $\partial\Omega \in C^3$ and specify time variable $t \in [0, T]$. Next, we supply the Cauchy problem by the appropriate b.c.
- $\varepsilon(x)$ and $\sigma(x)$ are dielectric permittivity and electric conductivity functions, respectively of the domain Ω . In (45), $\varepsilon(x) = \varepsilon_r(x)\varepsilon_0$, $\mu = \mu_r\mu_0$ and $\sigma(x)$ are dielectric permittivity, permeability and electric conductivity functions, respectively, ε_0, μ_0 are dielectric permittivity and permeability of free space, respectively.

Ω $\varepsilon_r(x) = ?$ $\sigma = 0, \mu_r = 1$ $E(x, t) = g(x, t)$ on $\partial\Omega$ Ω $\varepsilon_r(x) = ?$ $\sigma(x) = ?$ $\mu_r \approx 1$ $E(x, t) = g(x, t)$ on $\partial\Omega$

Inverse Problem (EIP1) Determine the relative dielectric permittivity function $\varepsilon_r(x)$ in Ω for $x \in \Omega$ in nonconductive ($\sigma(x) = 0$) and nonmagnetic ($\mu_r = 1$) media when the measured function $g(x, t)$ s.t.

$$\mathbf{E}(x, t) = g(x, t), \forall (x, t) \in \partial\Omega \times (0, T].$$

is known in Ω .

Inverse Problem (EIP2) Determine the functions $\varepsilon(x), \sigma(x)$ in Ω for $x \in \Omega$ for $\mu_r \approx 1$ in water assuming that $g(x, t)$ is known in $\partial\Omega \times (0, T]$.

CIPs for magnetic field

Similarly can be obtained Maxwell's equations for magnetic field $\mathbf{H} = (H_1, H_2, H_3)$. Let us consider system of Maxwell's equations in linear, isotropic, nondispersive, lossy materials with $\sigma = 0, \sigma^* = 0$:

$$\frac{\partial \mathbf{H}}{\partial t} = -\frac{1}{\mu} \nabla \times \mathbf{E} \quad (46)$$

$$\frac{\partial \mathbf{E}}{\partial t} = \frac{1}{\varepsilon} \nabla \times \mathbf{H} - \frac{1}{\varepsilon} \mathbf{J}_{source} \quad (47)$$

In this case we take time derivative in (46) and operator $\nabla \times$ in (47) to get:

$$\frac{\partial^2 \mathbf{H}}{\partial t^2} = -\frac{1}{\mu} \frac{\partial}{\partial t} \nabla \times \mathbf{E}, \quad (48)$$

$$\nabla \times \frac{\partial \mathbf{E}}{\partial t} = \nabla \times \frac{1}{\varepsilon} \nabla \times \mathbf{H} - \nabla \times \frac{1}{\varepsilon} \mathbf{J}_{source}. \quad (49)$$

Substitute the right hand side of (48) into (49) instead of $\frac{\partial}{\partial t} \nabla \times \mathbf{E}$ to obtain Maxwell's equations for magnetic field $\mathbf{H} = (H_1, H_2, H_3)$:

$$\mu \frac{\partial^2 \mathbf{H}}{\partial t^2} + \nabla \times \frac{1}{\varepsilon} \nabla \times \mathbf{H} = \nabla \times \frac{1}{\varepsilon} \mathbf{J}_{source} \quad (50)$$

Let us consider now Cauchy problem for magnetic field \mathbf{H} in the domain $\Omega_T = \Omega \times [0, T]$:

$$\begin{aligned} \mu \frac{\partial^2 \mathbf{H}}{\partial t^2} + \nabla \times \frac{1}{\varepsilon} \nabla \times \mathbf{H} &= \nabla \times \frac{1}{\varepsilon} \mathbf{J}_{source} \text{ in } \Omega_T, \\ \mathbf{H}(\mathbf{x}, \mathbf{0}) = f_0(x), \quad \mathbf{H}_t(\mathbf{x}, \mathbf{0}) &= f_1(x) \text{ in } \Omega, \end{aligned} \quad (51)$$

- Let $\Omega \subset \mathbb{R}^3$ be a convex bounded domain with the boundary $\partial\Omega \in C^3$ and specify time variable $t \in [0, T]$. Next, we supply the Cauchy problem by the appropriate b.c.
- In (51), $\varepsilon(x) = \varepsilon_r(x)\varepsilon_0, \mu = \mu_r\mu_0$ are dielectric permittivity and permeability functions, respectively, ε_0, μ_0 are dielectric permittivity and permeability of free space, respectively.

Different CIPs for time-dependent equation for magnetic field (51) can be formulated.

CIPs for magnetic wave propagation

 Ω

$$\mu_r(x) = ?$$

$$H(x, t) = g(x, t) \text{ on } \partial\Omega$$

 Ω

$$\begin{cases} \mu_r(x) = ? \\ \epsilon_r(x) = ? \end{cases}$$

$$H(x, t) = g(x, t) \text{ on } \partial\Omega$$

Inverse Problem (MIP1) Determine the relative magnetic permeability function $\mu_r(x)$ in Ω for $x \in \Omega$ in nonconductive ($\sigma(x) = 0$) media when the measured function $g(x, t)$ s.t.

$$\mathbf{H}(x, t) = g(x, t), \forall (x, t) \in \partial\Omega \times (0, T].$$

is known in Ω .

Inverse Problem (MIP2) Determine the functions $\epsilon_r(x), \mu_r(x)$ in Ω for $x \in \Omega$ assuming that $g(x, t)$ is known in $\partial\Omega \times (0, T]$.

Maxwell's equations in 2D in a waveguide. TE and TM modes.

Let us assume that the structure being modeled extends to infinity in the z-direction with no change in the shape or position of its transverse cross section (case of a waveguide). If the incident wave is also uniform in the z-direction, then all partial derivatives of the fields with respect to z must equal zero. Under these conditions, the full set of Maxwell's curl equations given by (28) and (29) reduces to

$$\frac{\partial H_x}{\partial t} = \frac{1}{\mu} \left[-\frac{\partial E_z}{\partial y} - (M_{source_x} + \sigma^* H_x) \right] \quad (52a)$$

$$\frac{\partial H_y}{\partial t} = \frac{1}{\mu} \left[\frac{\partial E_z}{\partial x} - (M_{source_y} + \sigma^* H_y) \right] \quad (52b)$$

$$\frac{\partial H_z}{\partial t} = \frac{1}{\mu} \left[\frac{\partial E_x}{\partial y} - \frac{\partial E_y}{\partial x} - (M_{source_z} + \sigma^* H_z) \right] \quad (52c)$$

$$\frac{\partial E_x}{\partial t} = \frac{1}{\varepsilon} \left[\frac{\partial H_z}{\partial y} - (J_{source_x} + \sigma E_x) \right] \quad (53a)$$

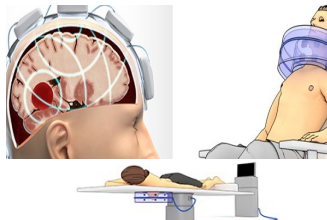
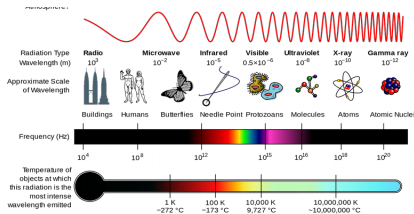
$$\frac{\partial E_y}{\partial t} = \frac{1}{\varepsilon} \left[-\frac{\partial H_z}{\partial x} - (J_{source_y} + \sigma E_y) \right] \quad (53b)$$

$$\frac{\partial E_z}{\partial t} = \frac{1}{\varepsilon} \left[\frac{\partial H_y}{\partial x} - \frac{\partial H_x}{\partial y} - (J_{source_z} + \sigma E_z) \right] \quad (53c)$$

If we will group (52a), (52b), and (53c), which involve only H_x , H_y , and E_z then we will set of field components to the *transverse-magnetic mode with respect to z (TM_z)* in two dimensions.

If we will group (53a), (53b), and (52c), which involve only E_x , E_y , and H_z . We shall designate this set of field components to the *transverse-electric mode with respect to z (TE_z)* in two dimensions.

Applications of CIPs for electric wave propagation



Left fig.: the electromagnetic spectrum (Wikipedia). Right fig.: Biomedical Microwave Imaging (frequencies around 1 GHz = 10^9 Hz) at the Department of Electrical Engineering at CTH, Chalmers, Göteborg, Sweden. Setup of Stroke Finder; microwave hyperthermia in cancer treatment and breast cancer detection, <https://www.chalmers.se/en/departments/e2/research/Signal-processing-and-Biomedical-engineering/>



Detection of explosives and airport security (usually X-ray technique) <https://www.rsdynamics.com/products/explosives-detectors/miniexplonix/>